MOLECULAR STRUCTURE AND INTERACTIONS OF NUCLEIC ACID COMPONENTS IN NANOPARTICLES: *AB INITIO* CALCULATIONS

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S u m m a r y

Self-associates of nucleic acid components (stacking trimers and tetramers of the base pairs of nucleic acids) and short fragments of nucleic acids are nanoparticles (linear sizes of these particles are more than 10 Å). Modern quantum-mechanical methods and softwares allow one to perform *ab initio* calculations of the systems consisting of 150–200 atoms with enough large basis sets (for example, 6-31G*). The aim of this work is to reveal the peculiarities of molecular and electronic structures, as well as the energy features of nanoparticles of nucleic acid components.

We had carried out *ab initio* calculations of the molecular structure and interactions in the stacking dimer, trimer, and tetramer of nucleic base pairs and in the stacking (TpG)(ApC) dimer and (TpGpC) (ApCpG) trimer of nucleotides, which are small DNA fragments.

The performed calculations of molecular structures of dimers and trimers of nucleotide pairs showed that the interplanar distance in the structures studied is equal to 3.2 Å on average, and the helical angle in a trimer is approximately equal to 30°. The distance between phosphor atoms in neighboring chains is 13.1 Å. For dimers and trimers under study, we calculated the horizontal interaction energies.

The analysis of interplanar distances and angles between nucleic bases and their pairs in the calculated short oligomers of nucleic acid base pairs (stacking dimer, trimer, and tetramer) has been carried out. Studies of interactions in the calculated short oligomers showed a considerable role of the cross interaction in the stabilization of the structures. The contribution of cross interactions to the horizontal interactions grows with the length of an oligomer. Nanoparticle components get electric charges in nanoparticles. Longwave low-intensity bands can appear in the electron spectra of nanoparticles.